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Abstract

This report concerns the energy of a zero-temperature many-body system of spin $\frac{1}{2}$ fermions interacting via a two-body potential with a free space infinite scattering length and zero effective range; the Unitary limit. Given the corresponding phase-shift $\delta(k) = \pi/2$ a one-term separable potential is obtained by inverse scattering assuming a momentum cut-off Λ such that $\delta(k) = 0$ for $k > \Lambda$. The *effective* interaction in the many-body system is calculated in a pp-ladder approximation with Pauli-blocking but neglecting mean-field (dispersion) corrections; effective mass $m^* = 1$. Using only the zero relative momentum component of this interaction the total energy is $\xi = 4/9$ (in units of the fermigas), a result reported by several previous authors. Integrating the momentum dependent interaction over the Fermi sea this energy is revised to $\xi = 0.24$. This result is independent of density and of the cut-off Λ if $\Lambda >\sim 3k_f$.

With $m^* \neq 1$ there is however a strong dependence on this cut-off.

Including hh-ladders estimates give $\xi = 0.4 \leftrightarrow 0.6$, but a reliable result would in this case require a Green's function calculation.

1 Introduction

The properties of a dilute fermigas with large scattering length is of considerable theoretical as well as experimental interest. Taking advantage of Feshbach resonances it is possible to magnetically tune the atomic scattering lengths, e.g.[1, 2, 3]. Increasing the scattering length of fermions from $-$ to $+\infty$ resulting in bound boson systems to explore the crossover from BCS to BEC has been reported by several groups.

A theoretically related problem proposed by George Bertsch [4] is that of the energy of a dilute system of spin 1/2 fermions interacting via a zero-range, infinite scattering length interaction referred to as the Unitary limit. For such a system one would expect the existence of a constant ξ being a function only of fundamental constants such that the total energy $E = \xi E_{FG}$ where E_{FG} is the uncorrelated Fermi-gas energy.

Several numerical methods have been used to determine ξ. The Monte Carlo calculations of Carlson et al.[5] are generally regarded to be the most complete and gives $\xi = 0.44 \pm 0.01$. The same (or similar) results are showm in refs. [6, 7, 8, 9] some of which are $\xi = 4/9$. Other authors report values of $\xi = 0.326$ [10, 11] while a recent result is $\xi = 0.25$[12].

It is a well-known fact that an interaction with large scattering length is separable. This paper is a report on results of calculations using a one term separable two-body interaction determined by inverse scattering from the phase-shift $\pi/2$, i.e. with infinite scattering length and zero effective range. It is shown in Section 2 that the calculations are greatly simplified in the Unitary limit with an effective mass $m^* = 1$.

Numerical results are shown in Section 3. In the limit when the Pauli blocking $Q \to 1$, the theory reduces to the phase-shift approximation as shown in Section 4. A comparison with some of the results of other authors is shown in Section 5 and a short summary with comments is found in Section 6.

2 Separable Interaction;Formalism

The use of a separable interaction in Nuclear Physics problems has a long history. It seems however that the first consistent calculation using inverse scattering techniques to construct a separable NN potential with an application to the nuclear matter problem was that reported in ref. [13]. A close agreement with calculations using the meson-theoretical potentials of Machleidt was found. Subsequent use was shown in ref. [14, 15] relating to V_{low-k} etc. In the latter of these two last references the dispersion corrections and its relation to saturation was of primary interest. It is well known that for a two-particle system with a bound state at or close to zero energy the interaction can be represented by a separable potential. The method described below in which this separable potential is obtained by inverse scattering is therefore suitable when considering the problem at hand, large scattering lengths. One of the main problems in an inverse scattering calculation is the change in sign of the phaseshift as a function of relative momentum. In the present case this is not an issue.

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A rank 1 separable potential provides a sufficient and in fact precise description of the interaction in the Unitary limit. It is assumed to be attractive and given by

$$V(k,p) = -v(k)v(p) \tag{1}$$

Inverse scattering then yields (e.g. ref [13, 16])

$$v^2(k) = \frac{(4\pi)^2}{k} sin\delta(k)|D(k^2)| \tag{2}$$

where

$$D(k^2) = exp\left[\frac{2}{\pi}\mathcal{P}\int_0^\Lambda \frac{k'\delta(k')}{k^2-k'^2}dk'\right] \tag{3}$$

where $\mathcal{P}$ denotes the principal value $\delta(k)$ the phaseshift. Λ provides a cut-off in momentum-space. The effect of the cut-off will be exploited below.

With $\delta(k) = \pi/2$ one finds

$$v^2(k) = -\frac{(4\pi)^2}{(\Lambda^2-k^2)^{\frac{1}{2}}} \tag{4}$$

and the interaction reduces to a constant for $\Lambda \gg k$, but $\to -\infty$ for $k \to \Lambda$.

The diagonal elements of the in-medium interaction is

$$G(k,P) = -\frac{v^2(k)}{1+I_G(k,P)} \tag{5}$$

with

$$I_G(k,P) = \frac{1}{(2\pi)^3}\int_0^\Lambda v^2(k')\frac{m^*Q(k',P)}{k^2-k'^2}k'^2dk' \tag{6}$$

where P is the center of mass momentum, Q the angle-averaged Pauli-operator for pp-ladders (Brueckner approximation) and m^* is the effective mass. One should note that the angle-averaging is exact in the effective mass approximation.

The divergence of $v^2(k)$ for large k indicated after eq.(4) makes the numerical integration in eq.(6) somewhat complicated. This can be overcome by the substitution $k' = \Lambda sin(t)$ to get

$$I_G(k,P) = \frac{1}{(2\pi)^3}\int_0^{\pi/2}\frac{m^*Q(\Lambda sin(t),P)sin^2tdt}{(k/\Lambda)^2-sin^2t} \tag{7}$$

The effective interaction $G(k,P)$ is in principle Λ-dependent. With $m^* = 1$ and $k/\Lambda \to 0$ and $Q \to 1$ for $\Lambda \gg k_f$, $I_G(k,P) \to -1 + \mathcal{O}(1/\Lambda)$. With $v^2(k) \to 1/\Lambda$ one therefore finds $G(k,P)$ independent of Λ for large Λ. If on the other hand one sets $1/\Lambda = 0$ in eq. (7) then $G \equiv K$, where K is the reactance matrix as defined below.

The (in)dependence of Λ is more clearly seen by using the following method applicable with $m^* = 1$. One should note that both of the eqs (6) and (7) involve integrations up to Λ. A regularization that restricts the momentum-integration in eq. (6) to momenta $\leq 2k_f$ can be achieved as follows.

With a separable interaction the Reactance-matrix K is defined by

$$K(k) = -\frac{v^2(k)}{1+I_K(k)} \tag{8}$$

with

$$I_K(k) = \frac{1}{(2\pi)^3}\int v^2(k')\frac{\mathcal{P}}{k^2-k'^2}k'^2dk' \tag{9}$$

where $\mathcal{P}$ refers to a principal value integration. Therefore K is real and its on-shell diagonal component is given by

$$K(k) = -4\pi tan\delta(k)/k. \tag{10}$$

In the Unitary case with $\delta(k) = \pi/2$, $K(k) \to \infty$, implying $I_K(k) = -1$. As stated above this is consistent with eq. (7) which for $Q = 1$ and $m^* = 1$ also results in $I_G = -1$ independent of $k < \Lambda$.

Eqs (5) and (8) can be combined to get [2]

$$G(k,P) = -\frac{v^2(k)}{I_{GK}(k,P)} \tag{11}$$

with

$$I_{GK}(k,P) = \frac{1}{(2\pi)^3}\int v^2(k')\frac{Q(k',P)-\mathcal{P}}{k^2-k'^2+i\eta}k'^2dk' + \frac{kv^2(k)}{tan\delta(k)} \tag{12}$$

The resulting form, eq.(11) is very suitable for the problem at hand because in the unitary limit the last term in eq. (12) $\to 0$. Furthermore, $Q \to 1$ for $k' > 2k_f$. The summation (integration) over intermediate states in eq. (12) therefore only involves momenta $\leq 2k_f$. One should observe that with Q defined for pp-ladders, I_{GK} is real for $k < k_f$ which is the case here. With hh-ladders one has pole-terms contributing to imaginary parts.

Note that this regularization of the G-matrix equation is possible only because of the neglect of the dispersion correction i.e. with $m^* = 1$.

As shown by eq. (4), $v(k)$ is constant to any desired accuracy for momenta $k \leq 2k_f$ by choosing Λ large enough. Equation (11) then simplifies. It is independent of the interaction because one can set $v(k) = v(k')$. The momentum-integration can then be done analytically as shown below. This simplification is not possible if using eq. (6) with integration up to the cut-off Λ where the interaction (4) diverges. It is also simpler than although in principle equivalent to eq. (7).

As stated above, the Reactance matrix is real and so is the G-matrix (for occupied states) when defined with pp-ladders like in Brueckner theory. After dividing by $v^2(k') = v^2k$ in eq. (12) the integral is conveniently evaluated analytically One finds with $a = \frac{k}{k_f}$ and $y = \frac{P}{2k_f}$:

$$I_{GK}(a,y) = \frac{k_f}{\pi}\left[1+y+a*log\left|\frac{1+y-a}{1+y+a}\right| + \frac{1}{2y}(1-y^2-a^2)log\left|\frac{(1+y)^2-a^2}{1-y^2-a^2}\right|\right] + kcot\delta(k). \tag{13}$$

To include hh-ladders there is an additional term

$$I_{hh}(a,y) = \frac{k_f}{\pi}\left[2(1-y^2)^{\frac{1}{2}} + a*log\left|\frac{(1-y^2)^{\frac{1}{2}}-a}{(1-y^2)^{\frac{1}{2}}+a}\right|\right]. \tag{14}$$

The diagonal G-matrix elements are

$$G(a,y) = -4\pi[I_{GK}(a,y) - \frac{1}{a_s} + \frac{1}{2}r_0k^2]^{-1} \tag{15}$$

where the two terms with scattering length a_s and effective range r_0 drop out in the unitary limit but kept here for a discussion in Sect (5).

With $G(a,y)$ given, the potential energy per particle PE/A is

$$PE/A = \frac{3k_f^3}{\pi^2}\int_0^1\left[\int_0^{1-a}8G(a,y)y^2dy + \frac{1}{a}\int_{1-a}^{(1-a^2)^{\frac{1}{2}}}4G(a,y)(1-y^2-a^2)ydy\right]a^2da \tag{16}$$

The kinetic energy per particle, i.e. the uncorrelated fermi-gas energy is given by

$$E_{FG}/A = \frac{3}{10}\frac{\hbar^2}{m}k_f^2.$$

The total energy is expressed in these units by

$$E/A = \xi E_{FG}/A.$$

[2] This is a somewhat similar subtraction method as used to get eq. V(34) in ref.([17]) and also used by S.A. Moszkowski in unpublished work [9].

3 Numerical Results

All results are for allowing the scattering length $a_s \to \infty$ and effective range $r_0 = 0$. The integral $I(a, y) = 0$ (i.e. $G \to \infty$) along a line $y = f(a)$ in the (a, y)-plane from approximately $(0.84, 0)$ to approximately $(0.90, 0.30)$. This complicates the numerical evaluation of the potential energy. This line is first extracted numerically by iteration at each meshpoint of the variable a to find $f(a)$. The function $I(a, y)$ is fitted to second order in y for each value of a in some interval Δy across this line $f(a)$. The same techniques as used in standard principal value integrations is then used together with a shift in meshes so that one point will be located on the line $f(a)$.

The momentum-integration leading to the effective interaction was calculated analytically using eq. (13) and also numerically from eq. (7) (with the same result). The integrations for PE/A, eq. (16), were done numerically. The result independent of density is

$$\xi = 0.24.$$

It may be of some interest to see some results of approximations. So for example with

$$I(a, y) \to I(0, 0) = -\frac{2k_f}{4\pi^2}$$

one finds

$$\xi = 4/9$$

which is a result also obtained by Steele [7] in the same approximation, but quite different from our $\xi = 0.24$. If on the other hand one allows for a dependence on center of mass momentum by using $I(o, y)$ one finds

$$\xi = 0.515.$$

One has to conclude that the momentum dependence on the effective interaction $G(k, P)$ cannot be ignored when calculating the energy of the many-body system.

The above results are were obtained with a summation over pp-ladders as in Brueckner theory. One may inquiry as to the importance of hh-ladders for the present problem. By redefining the Q-operator by using

$$Q = 1 - n_1 - n_2$$

instead of $Q = (1 - n_1)(1 - n_2)$ (n being occupation-numbers) in the above equations one finds

$$\xi = 0.4 \leftrightarrow 0.6.$$

The uncertainty in the results is related to the pairing instability. Experience from nuclear matter calculations appears to be that this is to a large extent resolved by the Green's function method with integrations over the energy variable in the spectral functions. The above estimate of including the hh-ladders cannot be considered meaningful. A Green's function calculation is necessary in this case; results will be presented in a forthcoming report.

To some approximation one might expect the pp- and hh-ladder contributions to be equal. This assumption was used in ref.[10]. Doing so here one finds

$$\xi = 0.56.$$

But again, this result is not reliable.

The convergence of $G(k, P)$ when increasing Λ is not obvious from eqs (5-7). These eqs are however equivalent with eqs (11,12) which clearly do converge. That these two set of equations are indeed equivalent was also found numerically. But the last set of equations assume that $m^* = 1$. It is found from numerical tests that eqs (5-7) do not converge with increasing Λ so the problem with $m^* \neq 1$ is not resolved here. As an example it is found that with $m^* = 0.9$, $\xi \to 1$ as $\Lambda \to 10^3 k_f$.

4 $Q \to 1$; The Phase-shift approximation

Two particles in a large box can be considered a limiting case of a many-body system. The effective interaction between two particles in a box having a relative momentum k is known to be given by [18, 19, 20, 21, 22]

$$G(k) = -4\pi\delta(k)/k.$$

It is reasonable to expect a proper many-body theory of effective interactions to give this result in the limit $Q \to 1$. This limit has to be taken with caution. If one simply lets $Q \to 1$ in eq. (12) and then takes the principal value one finds

$$I_{GK} = \frac{kv^2(k)}{tan\delta(k)}$$

and

$$G_{Q\to 1}(k) = -4\pi tan\delta(k)/k \equiv K(k)$$

where $K(k)$ was defined by eq. (10) that relates to the *free* scattering of two particles rather than two particles in a box. (If instead inserting an $i\eta$ in the denominator one obtains the complex T-matrix.) The correct limit is obtained after realising that when studying a many-body system one has to explicitly consider an enclosure of the particles in a large but finite box with a disrete rather than continuous spectrum. When extending the system so that sums can be replaced by integrations the transition from the discrete problem to the continuous has to be done with care. It has been shown [18, 19, 20] that when taking the limit $Q \to 1$ one should in this case use

$$\frac{1}{e} \to \frac{\mathcal{P}}{e} + \gamma$$

with

$$\gamma = k(\frac{1}{\delta(k)} - \frac{1}{tan\delta(k)}).$$

Doing so in eq. (12) one finds correctly

$$G_{Q\to 1}(k) = -4\pi\delta(k)/k.$$

This may serve as a test of the equations. It was used in early work as an approximation to $G(k)$ and referred to as the *phase-shift approximation* . It was believed to be a good approximation at low densities, substantiated by some numerical results. Of particular interest in relation to the Unitary problem is that it was used to calculate the binding energy for a neutron-gas at low density [23, 24]. In this approximation of the effective two-body in-medium interaction one finds with $\delta(k) = \frac{\pi}{2}$, $PE/A = -4/3E_{FG}$ giving

$$\xi = -\frac{1}{3}$$

quite different from any other result suggesting it to be a poor approximation here. The effect of the Pauli-blocking was however also calculated in ref.[24]. (The total energy of the neutron-gas reported there is some 20% lower than reported in recent publications[25].) Contrary to other beliefs the potential energy was found to be over-estimated by the phase-shift approximation by a factor varying between $1.75 - 1.95$ for $0.1fm^{-1} \geq k_f \leq 0.5fm^{-1}$. These results were obtained with $^1S_0$ phase-shifts and would not be directly applicable to the problem at hand. Using the same correction for the present Unitary problem would however give $PE/A = (-0.76 \leftrightarrow -0.68)E_{FG}$ and

$$\xi = 0.24 \leftrightarrow 0.32$$

in fair agreement with our result $\xi = 0.24$.

5 Comparison with previous work

The first publication relevant for comparing with the present work appears to be that of Baker[11]. He considered an attractive square-well potential with a radius $c \to 0$ and an extrapolation of scattering length $a \to -\infty$. The energy of the system was calculated in a pp-ladder approximation similar to the Brueckner G-matrix as used in the present report. It is however modified to avoid the Emery singularities [26]. The numerical evaluation of the energy using this 'R'-matrix gives a divergent result for $k_F c \to 0$ present at all scattering lengths. A Padé approximant gave $\xi \sim 0.40$. Baker also provides a series expansion of the ladder sum for $c = 0$. A [2/2] Padé approximant of this sum gives $\xi = 0.568$ while the [1/1] gives $\xi = 0.326$.

Heiselberg [10] has made extensive calculations both using a Galitskii resummation of hh- and pp-ladders resulting in $\xi = 0.33$ and in a low order variational caculation resulting in $\xi = 0.46$. The Galitskii method is somewhat similar to the present. One difference is that an average momentum was used when calculating the energy. As already mentioned above the hh- and pp-contribution were assumed to be equal which is another approximation.

The Monte Carlo calculations of Carlson et al[5] find a large pairing gap and a $\xi = 0.44 \pm 0.01$ including the pairing contributions. Without a pairing trial function (using a Slater determinant) they obtain $\xi = 0.54$. [3]

Eq. (13) for $I_{GK}(a, y)$ is the same function as $f(\kappa, s)$ (except for the *cot*-term) in the report by Steele, although with at least formally a very different method, using Effective Field Theory and Power Counting. [7] The expression for the potential energy (16) is consequently (in the limit of large sacttering length and with pp-ladders) also equal to that of Steele's. In his eq. (27) he lets $f(\kappa, s) \to 2$ which is equivalent to our $I(0, 0) = \frac{2k_f}{\pi}$ already considered as an approximation in Sect. 3. In this limit our results conequently agree giving $\xi = 4/9$. This result is also obtained by Moszkowski[9]. Within the framework of Steele's work his approximation $f(\kappa, s) \to 2$ seems formally consistent with his expansion to order $1/\mathcal{D}$. In the present work there is however no expansion other than in Λ and a_s and the integrations over (a, y) gives a substantial correction from $\xi = 4/9$ to $\xi = 0.24$.

Chen [8] like several other autors, finds $\xi = 4/9$ but only in a low density expansion. He uses a relativstic approach motivated by the analogy with the infrared limit of Coulomb correlations. In the non-relativstic limit he finds the energy per particle to be a function of k_f .

Our result with pp-ladders, $\xi = 0.24$ is appreciably smaller than in most reports. As mentioned in Sect. 4 it is to some extent substantiated by comparison with the neutron-gas calculations in ref. [24]. The calculations of Carlson et al[5] suggest that the pairing correction would give an even smaller ξ. The theoretical value closest to our result appears to be that of Lee[12] who calculated ξ on the lattice with 22 particles in a periodic cube and found $\xi = 0.25(3)$. The estimate alluded to in Sect. 3 including the hh-ladders giving

$$\xi = 0.4 \leftrightarrow 0.6$$

lies in the range of most of the results but needs a better treatment by Green's function methods.

There are experimental results reported between $\xi = 0.74 \pm 0.07$[2] and $\xi = 0.32^{+0.13}_{-0.10}$[3].

6 Summary and discussion

This work addresses the problem of the energy of a zero temperature fermion gas in the unitary limit. The free-space two-body interaction is assumed to be separable. This assumption should in itself not affect the results that are expected to be independent of the shape or strength of the interaction defined only by the scattering length and effective range. The details of the interaction does not otherwise enter explicitly into the expression for the effective interaction or many-body energy. The separable interaction was in eqs. (1-4) determined by inverse scattering. Eq. (4) showed explicitly that in the unitary limit, $a_s \to \infty$ and $r_0 \to 0$ the interaction is constant, independent of momenta for $k \ll \Lambda$. As Λ can be chosen arbitrarly large the interaction can then, with any chosen accuracy be considered a constant for all $k \leq 2k_f$, $2k_f$ being the maximum relative momentum in $Q - 1$ in eq. (12). To perform the calculation of ξ in the Unitary limit the effective interaction G can therefore be *chosen* to be independent of the interaction.

The terms with a_s and r_0 in eq. (15) do depend on the interaction. This equation would only be approximate for finite values of these quantities and justified only to the degree that the interaction $v(k)$ is constant. Numerical solution of eqs (1-3) shows that a necessary condition is that, as expected, $r_0 = 0$.

The calculations are mainly analytical. The numerical integrations are simple. The result is as expected for a unitary limit independent of the assumed shape or strength of the interaction as well as of the density. The assumption of infinite scattering length sets the scale.

The expression in eq. (16) for the potential energy agrees with that of Steele[7] using an EFT method and powercounting. This is not circumstantial, but ceratinly rooted in the fact that both methods, the separable potential and the EFT-power-counting rely on the nearly bound state with a pole near the real axis. There is a difference in final result in that the calculation here is carried a step further by doing the momentum integrations over occupied states.

A selfconsistent inclusion of the hh- ladders and the related effect of spectral widths would be achieved in a Green's function calculation. In nuclear matter calculations these effects are found to be repulsive relative to the Brueckner results that include only pp-ladders with the potential energy increased by $\sim 8\%$.[27] Applying such a correction here results in $\xi \sim 0.3$.

Green's function methods will be used in a forth-coming report on spectral functions and densities in momentum space.

[3] I am indebted to K.E. Schmidt to point this out to me.

There does not seem to be a consensus within the different theoretical calculations. It would be expected that the most accurate are those of Carlson et al [5]. The result of the present investigation does not support those findings.

The results within the present formalism are independent of density. This is expected to be general in the Unitary limit. At higher densities traditional many body theories predict higher order diagrams such as propagator modification by the mean field, included in standard Brueckner calculations to become important and. It is not clear how to deal with these problems in the Unitary limit.

An example of such a problem is the effective mass. All calculations here are with $m^* = 1$. The formalism used in the present calculations only works for this case. It is found however that the mean field is practically independent of momentum so that $m^* = 1$ is realistic.

BCS-pairing has not been included here. It is expected to lead to important corrections. Superfluid gaps have been calculated [10] and are large for $k_F a > 1$. QMC calculations show ξ to decrease by about 0.1 when BCS-correlations are included in the trial wave-function [5].

The rather different results obtained for the coefficient ξ in the Unitary limit both in experimental as well as theoretical reports suggests that this problem is still not resolved.

It is somewhat intriguing that although ξ is expected to be a universal constant its theoretical determination requires relatively complicated calculations. It is true that some estimates such as $\xi = 4/9$ are the result of very simple assumptions and agree closely with the supposedly most accurate determination, ref [5]. Closer examination seem to suggest however (as in the present investigation) that these simple assumptions are not valid.

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